Classical Mechanics and Quantum Mechanics

Review of Fundamentals of Classical Mechanics (Canonical Formalism):

- Canonical variables q_i, p_i
  A complete description of physical system
- Hamiltonian $H(q,p,t)$ determines dynamics (time-evolution)
- Least Action Principle $\delta\left[\int [p_i \dot{q}_i - H(q,p,t)]dt\right] = 0$ i.e. $\delta S_H = 0$
- Canonical Eqns $\dot{q}_i = \frac{\partial H}{\partial p_i}$; $\dot{p}_i = -\frac{\partial H}{\partial q_i}$
  (Central Problem: Integrate these eqns)
- Dynamical variables $A(q,p,t)$
- Poisson Bracket $[A,B]$ – Lie Algebra structure for dynamical variables. These can be derived from canonical brackets $0 = [q_i, q_j] = [p_i, p_j]$; $[q_i, p_j] = \delta_{ij}$
- Time evolution of dynamical variable:
  $$\frac{dA}{dt} = [A,H] + \frac{\partial A}{\partial t}$$
- Canonical Transformation $H, q, p \to K, Q, P$
  $\dot{Q}_i = \frac{\partial K}{\partial P_i}$ $\dot{P}_i = -\frac{\partial K}{\partial Q_i}$ $[Q_i, P_j] = \delta_{ij}$ etc--
- $G_2(q,P,t)$: $p_i = \partial G_2/\partial q_i$, $Q_i = \partial G_2/\partial P_i$, $K = H + \partial G_2/\partial t$
- Infinitesimal Canonical Transformation
  – Generated by $G^*(q,p,t)$; $\delta A = \epsilon[A, G^*]$
  (Time evolution is a canonical trans generated by H)
- Symmetries
  Inf canon. trans. generated by $G^*(q,p)$ leaves H invariant
  $[H, G^*] = 0 \Longrightarrow G^*$ is conserved
- H-J theory:
  If $\frac{\partial}{\partial t} S(q,t) + H(q, \frac{\partial S}{\partial q}, t) = 0$, then
  S generated canonical trans such that Q, P are constant
  (S = action as function of the coordinates)
- separable problems + action-angle variables
  Multiply periodic N Torus in 2N dim phase space
- No of one-valued constants of motion $\Longrightarrow$
  2N minus dimensionality of system manifold

Fundamentals of Quantum Mechanics (canonical Quantization):
(Given classical system, how do we quantize it?)

- Hilbert Space: (complete) complex inner-product space, the arena of QM $(\phi, \psi) = (\psi, \phi)^* = \phi_1^* \psi_1 + \phi_2^* \psi_2 + \dots$

- States of a QM system = rays in Hilbert space $\vec{\psi}$ with unit length, arbitrary phase

- Observable (dynamical variable) is a hermitian linear (actually self-adjoint) operator in Hilbert space
  E.g. $\underset{\sim}{q}, \underset{\sim}{p}$

  What is the connection of these operators to outcome of a measurement?

  Observable $\underset{\sim}{A}$ has basis of eigenvalues $\underset{\sim}{A} v_a = \lambda_a v_a$

  $\psi = \sum_a \psi_a v_a \quad . \quad \sum_a |\psi_a|^2 = 1$

  Then if $\underset{\sim}{A}$ is measured for state ψ. $|\psi_a|^2$ is probability that outcome is λ_a.

  In state $\vec{\psi}$, expectation value of $\underset{\sim}{A}$ is

  $\langle \underset{\sim}{A} \rangle = \sum_a \lambda_a |\psi_a|^2 = (\vec{\psi}, \underset{\sim}{A} \vec{\psi})$

- Dynamics is determined by $H(\underset{\sim}{q}, \underset{\sim}{p})$
  To explain how we must first consider ordering of operators

- Commutators (Canonical Quantization)
  operators (e.g. matrices) do not commute. How do we assign commutators when we want to quantize a system?

$$[\underset{\sim}{A}, \underset{\sim}{B}]_{com} \equiv \underset{\sim}{A}\,\underset{\sim}{B} - \underset{\sim}{B}\,\underset{\sim}{A} = ?$$

Note that $[\ ]_{com}$ has same algebraic properties as $[\ ]_{P.B.}$

1) $[\underset{\sim}{A}, \underset{\sim}{B}]_{com} = -[\underset{\sim}{B}, \underset{\sim}{A}]_{com}$

2) $[a\underset{\sim}{A} + b\underset{\sim}{B}, \underset{\sim}{C}]_{com} = a[\underset{\sim}{A}, \underset{\sim}{C}] + b[\underset{\sim}{B}, \underset{\sim}{C}]$

3) $[\underset{\sim}{A}\,\underset{\sim}{B}, \underset{\sim}{C}]_{com} = \underset{\sim}{A}[\underset{\sim}{B}, \underset{\sim}{C}]_{com} + [\underset{\sim}{A}, \underset{\sim}{C}]_{com}\underset{\sim}{B}$

4) $[[\underset{\sim}{A}, \underset{\sim}{B}]\underset{\sim}{C}] + [[\underset{\sim}{C}, \underset{\sim}{A}]\underset{\sim}{B}] + [[\underset{\sim}{B}, \underset{\sim}{C}]\underset{\sim}{A}] = 0$

(Lie Algebra of Observables)

It is consistent to assign commutators in the following way: Suppose $\underset{\sim}{A}(\underset{\sim}{q}, \underset{\sim}{p})$ is the same function of $\underset{\sim}{q}, \underset{\sim}{p}$ that $A(q,p)$ is of q,p, and similar for $\underset{\sim}{B}$, $\underset{\sim}{C}$ etc

Then, if $\boxed{[A, B]_{P.B.} = C, \text{ assign } [\underset{\sim}{A}, \underset{\sim}{B}] = i\hbar\underset{\sim}{C}}$

$\hbar$ = Planck's constant

This is consistent because both brackets obey rules (1)-(3) above. Hence any bracket can be reduced to the canonical brackets, e.g.

$$[\underset{\sim}{p}_i, \underset{\sim}{q}_i] = -i\hbar\mathbf{I} \quad \text{etc..}$$

Tells us $\Rightarrow$ Hilbert space must be ∞ dimensional

(One must be cautious about ordering ambiguities, however – e.g. $qp \to \frac{1}{2}(\underset{\sim}{q}\underset{\sim}{p} + \underset{\sim}{p}\underset{\sim}{q})$: hermitian)

It really suffices to specify

$$\boxed{[\underset{\sim}{q}_i, \underset{\sim}{q}_j] = 0 \quad [\underset{\sim}{p}_i, \underset{\sim}{p}_j] = 0 \quad [\underset{\sim}{q}_i, \underset{\sim}{p}_j] = i\hbar\,\delta_{ij}}$$

These canonical commutation relations completely define the quantum mechanical system.

As $\hbar \to 0$, all observables commute

- Time Evolution

when we carry out canonical quantization, the Hamiltonian of the QM system becomes
$\underset{\sim}{H}(\underset{\sim}{q}, \underset{\sim}{P})$

the classical eqn $\frac{dA}{dt} = [A, H]_{P.B.}$ (time-independent dynamical variable)

suggests $\boxed{i\hbar \frac{d}{dt} \underset{\sim}{A} = [\underset{\sim}{A}, \underset{\sim}{H}]_{com}}$ (Heisenberg picture dynamics)

the "correspondence principle" is built into this relation, because, if we take expectation values

$$i\hbar \frac{d}{dt}\langle \underset{\sim}{A} \rangle = \langle [\underset{\sim}{A}, \underset{\sim}{H}] \rangle = i\hbar \langle \underset{\sim}{C} \rangle$$

where $C = [A, H]_{P.B.}$

Thus, the expectation values of observables evolve like classical dynamical variables.

- Unitary Transformations

$\underset{\sim}{Q} = \underset{\sim}{U}\,\underset{\sim}{q}\,\underset{\sim}{U}^{+}$ $\quad \underset{\sim}{U}\underset{\sim}{U}^{+} = \underset{\sim}{\mathbb{1}}$ $\quad$ (Hermitian → Hermitian)

$[\underset{\sim}{Q}, \underset{\sim}{P}]_{com} = \underset{\sim}{U}[\underset{\sim}{q}, \underset{\sim}{p}]\underset{\sim}{U}^{+} = i\hbar$

transformation is "canonical" - it preserves all poisson brackets (canonical commutators)

[One can also prove converse: If $\underset{\sim}{Q}, \underset{\sim}{P}$ obey canonical relations, there is a unitary trans taking $\underset{\sim}{q}, \underset{\sim}{P}$ to $\underset{\sim}{Q}, \underset{\sim}{P}$. See Dirac, Principles of QM]

All reps of ~~comm.~~ relations unitarily equivalent - Von Neumann

- Infinitesimal Unitary Transformation

$\underset{\sim}{U} = \underset{\sim}{\mathbb{1}} + i\epsilon \underset{\sim}{G}$ $\quad \underset{\sim}{U}\underset{\sim}{U}^{+} = \underset{\sim}{\mathbb{1}} = \underset{\sim}{\mathbb{1}} + i\epsilon(\underset{\sim}{G} - \underset{\sim}{G}^{+})$

$\underset{\sim}{U}^{+} = \underset{\sim}{\mathbb{1}} - i\epsilon \underset{\sim}{G}^{+}$ $\quad \Longrightarrow \underset{\sim}{G} = \underset{\sim}{G}^{+}$

Inf unitary transformations are generated by observables (self-adjoint operators)

$$A \to UAU^\dagger = A + i\epsilon[G, A]$$

Note: time evolution is a unitary trans generated by the Hamiltonian

If $[G, H] = 0$, then unitary trans. generated by G leaves H invariant (symmetry) and $\frac{d}{dt}G = 0$

- Schrodinger Eqn

If H is not explicitly time-dependent, the canonical transformation which "stops" the motion of an observable is

$$U(t) = e^{-iHt/\hbar} \qquad U^\dagger(t) = e^{iHt/\hbar}$$

$$\frac{d}{dt}U(t) = \frac{1}{i\hbar}HU = \frac{1}{i\hbar}UH$$

$$\frac{d}{dt}A' = \frac{d}{dt}UAU^\dagger = \frac{1}{i\hbar}U\left[[A, H] + HA - AH\right]U^\dagger = 0$$

But holding observables fixed causes states to move

$$\vec{\Psi} = U(t)\vec{\Psi}_0 \Rightarrow \boxed{\frac{d}{dt}\vec{\Psi} = \frac{1}{i\hbar}H\vec{\Psi}}$$ Schrödinger Eqn

- Schrödinger Representation

Represent Hilbert Space by functions of the q_i

$$\Psi(q_1, \ldots q_N, t)$$

(Recall: all reps are equivalent)
– Inf dimensional space required, as is clear from comm. relations)

then q_i is multiplication by q_i

p_i is $-i\hbar\frac{\partial}{\partial q_i}$ – gradient

$$[q_i, p_j] = -\left(-i\hbar\frac{\partial}{\partial q_j}\right)q_i = i\hbar\delta_{ij}$$

E.g., for a particle in a potential $H = \frac{\vec{p}^2}{2m} + V(\vec{x})$

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x})$$

Schrodinger Equation and Hamilton Jacobi Theory

$$i\hbar \frac{\partial}{\partial t}\psi = \underset{\sim}{H}(\underset{\sim}{q}, \underset{\sim}{p})\psi \qquad \psi = \psi(q,t)$$

Represent $\psi = e^{iS/\hbar}$

$$i\hbar\left(\frac{i}{\hbar}\right)\frac{\partial S}{\partial t} e^{iS/\hbar} = \underset{\sim}{H} e^{iS/\hbar}$$

$$\Rightarrow \quad -\frac{\partial S}{\partial t} = e^{-iS/\hbar}\underset{\sim}{H} e^{iS/\hbar}$$

S is a function of q_i and $\underset{\sim}{p}_i = -i\hbar\frac{\partial}{\partial q_i}$

$$\Rightarrow \quad -\frac{\partial S}{\partial t} = H\left(q_i, -i\hbar\frac{\partial}{\partial q_i} + \frac{\partial S}{\partial q_i}\right)$$

Now, if we take formal $\hbar \to 0$ limit

$$\boxed{\frac{\partial S}{\partial t} + H\left(q_i, \frac{\partial S}{\partial q_i}\right) = 0}$$

the H-J eqn is the classical limit of the Schrodinger eqn

What approximation are we really making? Consider, for concreteness, the case of a particle in one dimension

$$H = p^2/2m + V(q)$$

$$0 = \frac{\partial S}{\partial t} + \frac{1}{2m}\underbrace{\left(-i\hbar\frac{\partial}{\partial q} + \frac{\partial S}{\partial q}\right)^2}_{\left(\frac{\partial S}{\partial q}\right)^2 - i\hbar\frac{\partial^2 S}{\partial q^2}} + V(q)$$

or

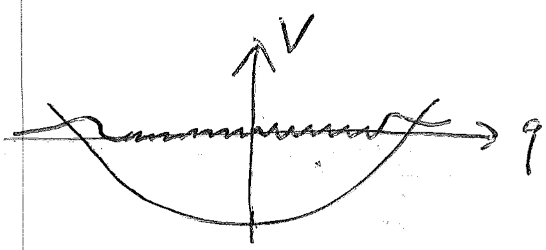
$$\text{or} \quad \boxed{\frac{\partial S}{\partial t} + \frac{1}{2m}\left(\frac{\partial S}{\partial q}\right)^2 + V(q) = \frac{i\hbar}{2m}\frac{\partial^2 S}{\partial q^2}}$$

We have to assume $\left(\frac{\partial S}{\partial q}\right)^2 \gg \hbar\left|\frac{\partial^2 S}{\partial q^2}\right|$

$$\text{or} \quad \frac{d}{dq}\left[\hbar\left(\frac{\partial S}{\partial q}\right)^{-1}\right] \ll 1$$

But H-J theory $\Rightarrow \frac{\partial S}{\partial q} = p$, so $\boxed{\frac{d}{dq}\left(\frac{\hbar}{p}\right) \ll 1}$

The <u>deBroglie wavelength</u> must change negligibly when q advances by one wavelength.



Thus, classical mechanics (H-J theory) is the short-wavelength (or "geometrical optics") limit of quantum mechanics. Another way of saying it is. $S/\hbar$, the phase of ψ, advances by a large amount when a small displacement is made

E.g. bacterium $m \sim 10^{-8}$ grams, $s \sim 10^{-3}$ cm, $t \sim 1$ sec

$$S = \tfrac{1}{2} m \left(\frac{s}{t}\right)^2 t = \tfrac{1}{2} 10^{-8} 10^{-6} = 5 \times 10^{-15} \text{ erg sec}$$

$$\hbar = 10^{-27} \text{ erg sec}$$

$$\Rightarrow \quad S/\hbar = 5 \times 10^{12}$$

Bacteria are classical

electron in atom $m \sim 10^{-27}$ g, $s \sim 10^{-8}$ cm, $v \sim 10^{+8}$ cm/sec

$$S = \tfrac{1}{2} 10^{-27} 10^{-8} 10^{+8} = \tfrac{1}{2} 10^{-27} \text{ erg sec}$$

$$S/\hbar = \tfrac{1}{2}$$

Electrons are quantum mechanical

Since $\psi \sim e^{iS_0/\hbar}$ where S_0 is the classical action

$\underset{m}{p}\,\psi = \dfrac{\partial S_0}{\partial q}\psi = p\,\psi$ – In the Schrodinger rep, $\underline{p}$, like q is just a multiplication operator

observables become numbers in the classical limit

The H-J theory is just the first term in a systematic expansion in powers of $\hbar$ for S. (called the "semiclassical" or "WKB" expansion)

$$S = S_0 + \frac{\hbar}{i} S_1 + \cdots \quad \text{or} \quad S = -Et + W_0 + \frac{\hbar}{i} W_1$$

Consider e.g. a particle in one-dimension. We know from solving the H-J eqn for

$$H = p^2/2m + V(q) \qquad [p(7.9)]$$

that

$$S_0 = \pm \int p\, dq - Et \qquad p = \sqrt{2m(E-V)}$$

W_0 = Hamilton's characteristic function = Maupertuis action

If we retain corrections of order $\hbar$ in the Schrodinger eqn,

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\left(\frac{\partial S}{\partial q}\right)^2 + V(q) = \frac{i\hbar}{2m}\frac{\partial^2 S}{\partial q^2}$$

$$\Rightarrow \quad \frac{1}{2m}\left(\frac{dW_0}{dq}\right)\left(\frac{dW_0}{dq} + 2\frac{\hbar}{i}\frac{dW_1}{dq}\right) + V - E = \frac{i\hbar}{2m}\frac{d^2W_0}{dq^2}$$

$$\Rightarrow \quad -p\frac{dW_1}{dq} = \frac{1}{2}\frac{dp}{dq}$$

$$dW_1 = -\frac{1}{2}\frac{dp}{p} \Rightarrow W_1 = -\frac{1}{2}\ln p + \text{const}$$

$$\exp(W_1) = C p^{-\frac{1}{2}}$$

$$\Rightarrow \quad \boxed{\psi = C p^{-\frac{1}{2}} \exp\left(\pm\frac{i}{\hbar}\int p\, dq\right)\left[1 + O(\hbar)\right] \times e^{-iEt/\hbar}}$$

The $p^{-\frac{1}{2}}$ is easy to interpret, since we have

$|\psi|^2 \propto \frac{1}{p} \propto \frac{1}{v}$ — this is the expected behavior for a classical trajectory

the probability $|\psi|^2 dq$ of finding particle between q and $q+dq$ is proportional to the time the classical particle spends there.

[To establish a connection between classical motion and the Schrodinger eqn, we need to construct narrow wave packets, and note that they evolve like classical particles, with negligible spreading of the packet for $\hbar$ sufficiently small.]

Note: Probability appears to diverge near endpoints: $\sim 1/v$. This is actually wrong; the quasiclassical approx always breaks down near the endpoints, because wavelength changes rapidly. The resolution of this problem is discussed in advanced QM texts, e.g. L+L.

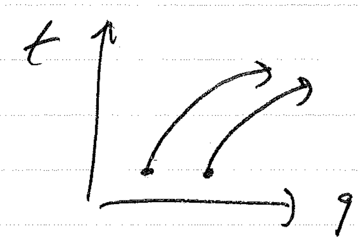
A further bonus: WKB works in classically forbidden regime

Propagation of a wave packet

Consider the particle in one dimension

$$\psi(q,t) \sim e^{i(\int p\,dq - Et)/\hbar}$$

If we consider a "surface of constant phase" we have $\quad p\,dq - E\,dt = 0$ or $\dfrac{dq}{dt} = E/p$



The surface of constant phase advance at a rate

$$v_{phase} = \frac{E}{p} \propto \frac{1}{v}$$

— inversely proportional to the classical velocity

To see the correspondence with classical motion more clearly, we should consider the evolution of a narrow wave packet

$$\psi(q,t) = \int dp\, \phi(p)\, e^{i(pq - E(p)t)/\hbar}$$

— where $\phi(p)$ is sharply peaked about $p = p_0$, with width $\sim \Delta p$

Expand E about p_0: $\quad E(p) = E_0 + (p-p_0)\dfrac{dE}{dp} + \frac{1}{2}(p-p_0)^2 \dfrac{d^2E}{dp^2} + \cdots$

$$= e^{i(p_0 q - E_0 t)/\hbar} \int dp\, \phi(p) \exp\left[i(p-p_0)\left(q - \frac{dE}{dp}t\right)/\hbar - \frac{1}{2}\frac{it}{\hbar}(p-p_0)^2 \frac{d^2E}{dp^2} + \cdots \right]$$

We can ignore higher order corrections in the exponent as long as

$$\frac{1}{\hbar}(\Delta p)^2 \frac{d^2E}{dp^2}\, t \ll 1$$

Then -- except for an overall phase

the wave form in q space is translated without changing shape

It moves according to

$$\Delta q = \frac{dE}{dp}\Delta t \quad \text{or} \quad \boxed{\dot{q} = \frac{\partial H}{\partial p}}$$

— Hamilton's equation

To understand the approximation

$v = \frac{dE}{dp} \Rightarrow$ there is velocity dispersion

$$\Delta v = \frac{d^2E}{dp^2}\Delta p$$

This leads to significant "spreading" of the wave packet after time t if

$t\Delta v \sim \Delta x$ or, from the uncertainty relation $\Delta x \sim \frac{\hbar}{\Delta p}$

This is $\frac{t}{\hbar}\Delta v\, \Delta p \sim 1$

or $(\Delta p)^2 \frac{d^2E}{dp^2}\, t/\hbar \sim 1$ -- So the condition found above is condition for spreading to be negligible

We can generalize this discussion to a general system with time independent Hamiltonian: Hamilton-Jacobi eqn is solved by

$$S = W(q) - Et$$

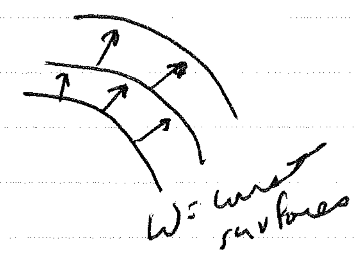
where $\dfrac{\partial W}{\partial q_i} = p_i$

Soln to Schrödinger eqn in geometrical optics is

$$\psi(q,t) \sim \exp[i(W(q) - Et)]$$

First consider surfaces of constant phase (in configuration space)

$$W(q) = Et + \text{constant}$$



Since $\vec{\nabla} W = \vec{p}$ -- and $\vec{\nabla} W$ is orthogonal to surfaces of constant W — we see that momentum points $\perp$ to surface of constant W

The rate at which this surface moves is

$$|\nabla W|(\Delta q) = E \Delta t \text{ or}$$

$$v_{phase} = \frac{E}{|\nabla W|} = \frac{E}{p}$$

But if we consider a wave packet, say of the form

$$\psi \sim \int dp\, \phi(p)\, e^{i(W(q) - Et)/\hbar}$$

— we again consider expanding around p_0 — where $\phi(p)$ is peaked

$$Et = E_0 t + (\vec{p} - \vec{p_0}) \cdot \vec{\nabla}_p E t$$

But we note that

$$W(\vec{q} + \delta\vec{q}) = W(\vec{q}) + \delta\vec{q} \cdot \vec{\nabla} W$$
$$= W(\vec{q}) + \vec{p} \cdot \delta\vec{q}$$

Thus — we can absorb the linear term in $(\vec{p} - \vec{p_0})$ into a shift in $\vec{q}$ by

$$\delta\vec{q} = \vec{\nabla}_p E \; t$$

Thus, the center of the wave packet propagates according to

$$\dot{q}_i = \frac{\partial}{\partial p_i} H \quad \text{— Hamilton's equation}$$

To see that the other Hamilton eqn is also satisfied, ~~we may appeal to the fact that the energy dispersion of the wave packet is negligible, and that energy is conserved, so that~~

$$\cancel{0 = \frac{\partial H}{\partial q_i} \dot{q}_i + \frac{\partial H}{}}$$

we could consider evolution of a wave packet in momentum space